

A data-driven test of a quantum-statistics PDF parametrisation

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based on work in collaboration with F.Buccella, F.Giuli and F.Tramontano



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To fit PDFs \rightarrow specify initial (low) scale Q_0 and PDF parametrisation

$$Q_0 \rightarrow f_i(x, Q_0^2, \{P\})$$

No analytical way to pick the initial parametrisation nor Q_0

- HERAPDF $\rightarrow f_i(x, Q_0^2) = x^\alpha(1-x)^\beta P_n(z)$ using polynomials [1506.06042]
- NNPDF $\rightarrow f_i(x, Q_0^2) = x^\alpha(1-x)^\beta \text{NN}(z)$ using neural networks [2109.02653]
- BG $\rightarrow f_i(x, Q_0^2) = x^\alpha(1-x)^\beta [P_n(z) + P_m(\log(z))]$ using $\log(z)$ polynomial for small- z region [1902.11125]
- ... many others [2207.04739],[1912.10053]

An alternative to a generic parametrisation is using physical arguments to model the structures of the proton...

Proton → gas mixture of massless partons **at equilibrium**

[1412.7683]

$$f^{\uparrow\downarrow}(E) = \frac{g_f V}{(2\pi)^3} \left[\exp\left(\frac{(E - \mu_f^{\uparrow\downarrow})}{T}\right) \pm 1 \right]^{-1},$$

In principle, constrain $\{V, T, \mu_f^{\uparrow\downarrow}\}$ using sum rules+maximising entropy

For a recent example

Phys. Lett. B 775 (2017) 172 – 177

Alternately, modify the distribution to build a PDF parametrisation

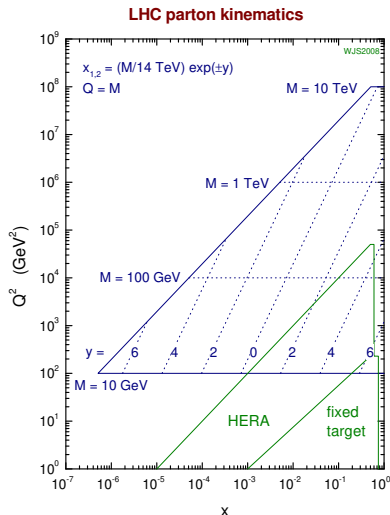
Proton → gas mixture of massless partons at equilibrium

[1412.7683]

- rewrite using dimensionless parameters

$$f_i^{\uparrow\downarrow}(x, Q_0^2) \supset \left[\exp\left(\frac{x - X_{0i}^{\uparrow\downarrow}}{\bar{x}}\right) \pm 1 \right]^{-1};$$

- “Chemical potentials” of quarks and antiquarks are related $X_{0q}^{\uparrow\downarrow} = -X_{0\bar{q}}^{\uparrow\downarrow}$
- Gluons behave like blackbody radiation → $X_{0g} = 0$
- Replace normalisation factor with $Ax^b X_{0i}^{\uparrow\downarrow}$ for quark
 $\bar{A}x^{\bar{b}}/X_{0i}^{\uparrow\downarrow}$ for antiquark
- sum rules should imply $u^\uparrow > d^\downarrow > u^\downarrow > d^\uparrow$ which would lead to $X_{0u}^\uparrow > X_{0d}^\downarrow > X_{0u}^\downarrow > X_{0d}^\uparrow$



Various determinations of QS PDF parameters in the literature

So far, determinations are mostly based on fits against public PDFs

[\[hep-ph/0109160\]](#) [\[1412.7683\]](#) [\[1502.02517\]](#) [\[2201.07640\]](#)

We want to perform a legitimate PDF fits to data using this QS parametrization

- to test the model
- (more important) to explore a new PDF parametrization depending on few parameters (useful e.g. for assessing parametrization bias)

We summarize the expressions from the model as

[1412.7683]

$$h(x; b, \bar{x}, X) = \frac{x^b}{\exp\left(\frac{x-X}{\bar{x}}\right) + 1},$$

$$xf_q^{\uparrow\downarrow}(x, Q_0^2) = AX_q^{\uparrow\downarrow} h\left(x; b, \bar{x}, X_q^{\uparrow\downarrow}\right) + \tilde{A}h\left(x; \tilde{b}, \bar{x}, 0\right), \quad (1a)$$

$$xf_{\bar{q}}^{\uparrow\downarrow}(x, Q_0^2) = \bar{A} \frac{1}{X_q^{\uparrow\downarrow}} h\left(x; \bar{b}, \bar{x}, -X_q^{\uparrow\downarrow}\right) + \tilde{A}h\left(x; \tilde{b}, \bar{x}, 0\right), \quad (1b)$$

with $q \in \{u, d\}$,

$$xf_g(x, Q_0^2) = \frac{A_g x^{b_g}}{\exp(x/\bar{x}) - 1}. \quad (1c)$$

An auxiliary “diffractive” term $\tilde{A}h(x; \tilde{b}, \bar{x}, 0)$ is introduced to control the high-energy region.

Fitting only unpolarised DIS data \rightarrow sum over helicity

$$f_q(x, Q_0^2) = f_q^{\uparrow}(x, Q_0^2) + f_q^{\downarrow}(x, Q_0^2)$$

Writing the unpolarised valence and sea contributions ($q \in \{u, d\}$)

$$\begin{aligned}
 x f_{q_v}(x, Q_0^2) &= q(x, Q_0^2) - \bar{q}(x, Q_0^2) \\
 &= A \left[X_q^\uparrow h(x; b, \bar{x}, X_q^\uparrow) + X_q^\downarrow h(x; b, \bar{x}, X_q^\downarrow) \right] \\
 &\quad - \bar{A} \left[\frac{1}{X_q^\downarrow} h(x; \bar{b}, \bar{x}, -X_q^\downarrow) + \frac{1}{X_q^\uparrow} h(x; \bar{b}, \bar{x}, -X_q^\uparrow) \right] \quad (2a)
 \end{aligned}$$

$$\begin{aligned}
 x f_{\bar{q}}(x, Q_0^2) &= \bar{A} \left[\frac{1}{X_q^\downarrow} h(x; \bar{b}, \bar{x}, -X_q^\downarrow) + \frac{1}{X_q^\uparrow} h(x; \bar{b}, \bar{x}, -X_q^\uparrow) \right] \\
 &\quad + 2\tilde{A} h(x; \tilde{b}, \bar{x}, 0), \quad (2b)
 \end{aligned}$$

$$x f_g(x, Q_0^2) = \frac{A_g x^{b_g}}{\exp(x/\bar{x}) - 1} \quad (2c)$$

$$s(x, Q_0^2) = \bar{s}(x, Q_0^2) = \frac{f_s}{1 - f_s} \bar{d}(x, Q_0^2) \quad \text{with} \quad f_s = 0.4. \quad (2d)$$

There are 13 parameters: $\{\bar{x}, A_g, A, \bar{A}, \tilde{A}, X_u^{\uparrow\downarrow}, X_d^{\uparrow\downarrow}, b, \bar{b}, b_g, \tilde{b}\}$

Additional constraints we apply:

- Valence and momentum **sum rules** \rightarrow fix normalisations $\{A_g, A, \bar{A}\}$
Valence sum rules require some care (A, \bar{A} are not overall factors) \rightarrow see later
- Regge theory + DGLAP imply that gluon and quark singlet behave the same at small x

$$x f_q(x, Q_0^2) \sim x^{\tilde{b}} \quad (3)$$

$$x f_g(x, Q_0^2) \sim x^{b_g - 1} \quad (4)$$

which implies the constraint

$$b_g = 1 + \tilde{b}$$

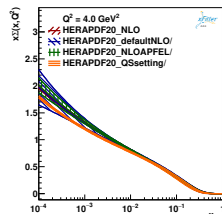
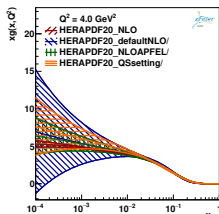
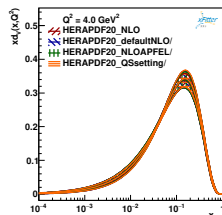
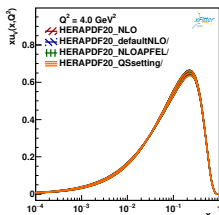
- We also fix $\tilde{b} = b$ for simplicity (further studies are ongoing)

This leaves 8 free parameters to fit: $\{\bar{x}, \tilde{A}, X_u^{\uparrow\downarrow}, X_d^{\uparrow\downarrow}, b, \tilde{b}\}$.

Potential bug found in NLO fit (gitlab master branch **84c362f1** 17/11/2022)

Legend:

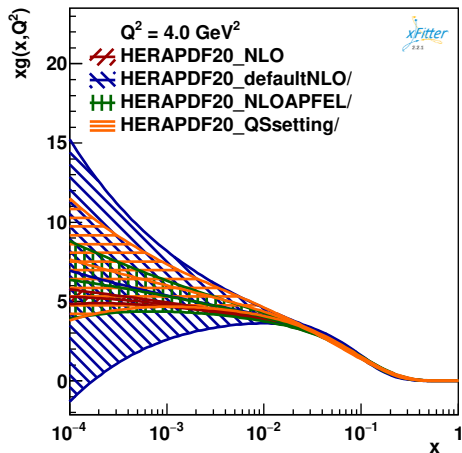
- **HERAPDF2.0_NLO** plot of the publicly available LHAPDF set
- **HERAPDF2.0_defaultNLO** output of the example in `xfitter`
- **HERAPDF2.0_NLOAPFEL** same as above, using different theory input
- **HERAPDF2.0_QSetting** benchmark for our parametrisation (wait next slides)



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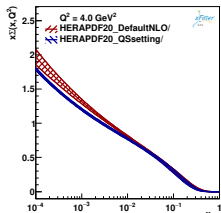
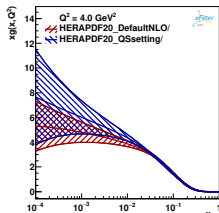
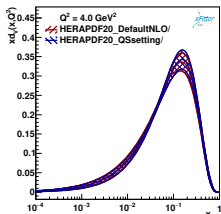
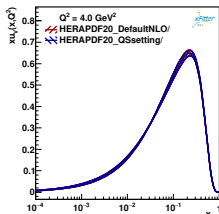
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Benchmark fit between default HERAPDF2.0 NLO configuration in `xfitter` and our settings

Some additional constraints are applied:

- Parametrisation scale
 $Q_0^2 = 4 \text{ GeV}^2$
→ we have to cut out the $Q^2 = 3.5 \text{ GeV}^2$ bin
- Theory inputs:
APFEL@NLO
VFNS (FONLL-B)



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- Improved description of
 NCep 920

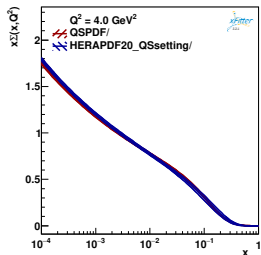
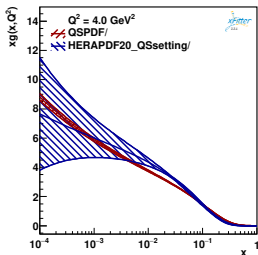
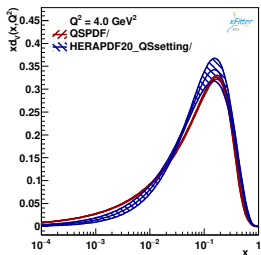
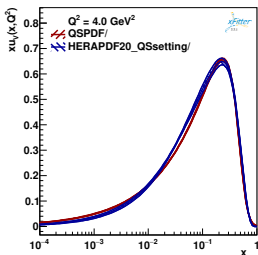
Dataset	HERAPDF20 Default- NLO	HERAPDF20 QSsetting	
HERA1+2 CCem	54 / 42	54 / 42	
HERA1+2 NCep 820	68 / 70	64 / 68	
HERA1+2 NCep 460	217 / 204	216 / 200	
\rightarrow HERA1+2 NCep 920	439 / 377	397 / 363	\leftarrow
HERA1+2 CCep	43 / 39	45 / 39	
HERA1+2 NCem	222 / 159	221 / 159	
HERA1+2 NCep 575	219 / 254	217 / 249	
Correlated χ^2	86	67	
Log penalty χ^2	+8.3	-4.68	
Total χ^2 / dof	1357 / 1131	1275 / 1106	
χ^2 p-value	0.00	0.00	

Testing the QSPDF parametrisation: fits and χ^2

Now we fit QSPDF against the HERA DIS dataset.

- Reduced error bands
- Only experimental uncertainty is accounted for

In **blue** the benchmark fit with the HERAPDF2.0 and in **red** the fit of QSPDF



Now we fit QSPDF against the HERA DIS dataset.

- Fit quality is good
- very minimal set of parametres

Dataset	QSPDF	HERAPDF20 QSsetting
HERA1+2 CCep	59 / 39	45 / 39
HERA1+2 CCem	69 / 42	54 / 42
HERA1+2 NCem	229 / 159	221 / 159
HERA1+2 NCep 820	71 / 68	64 / 68
HERA1+2 NCep 920	468 / 363	397 / 363
HERA1+2 NCep 460	231 / 200	216 / 200
HERA1+2 NCep 575	235 / 249	217 / 249
Correlated χ^2	104	67
Log penalty χ^2	-71.03	-4.68
Total χ^2 / dof	1397 / 1112	1275 / 1106
χ^2 p-value	0.00	0.00

	QSPDF	HERAPDF2.0
# param.	8	14
χ^2 /D.O.F.	1.26	1.15

Comparison with older determinations (not real fits to data)

[hep-ph/0109160]

We find:

- $X_u^\uparrow > X_d^\downarrow \sim X_u^\downarrow > X_d^\uparrow$
- Qualitative agreement determination of parameters
- No information on polarised PDF (unlike previous work)

Parameter	QSPDF	[hep-ph/0109160]
A	3.04	1.75
\bar{A}	0.12	1.91
A_g	33.52	14.28
\bar{A}	0.133 ± 0.004	0.083
X_d^\uparrow	0.14 ± 0.02	0.23
X_d^\downarrow	0.284 ± 0.007	0.302
X_u^\uparrow	0.419 ± 0.007	0.461
X_u^\downarrow	0.21 ± 0.02	0.298
$b = \bar{b}$	0.52 ± 0.01	0.41
$\tilde{b} = b_g - 1$	-0.173 ± 0.003	-0.253
\bar{x}	0.092 ± 0.001	0.099

Testing the QSPDF parametrisation: $\bar{d} - \bar{u}$ distribution

We compare the $\bar{d} - \bar{u}$ distributions explicitly
→ Interesting qualitative feature reproduced!

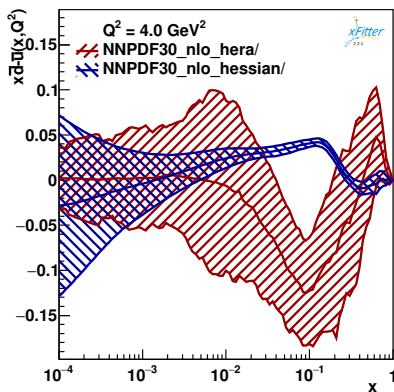


Figure: Comparison of NNPDF3.0 fits with the HERA dataset only and the default dataset, (NLO theory)

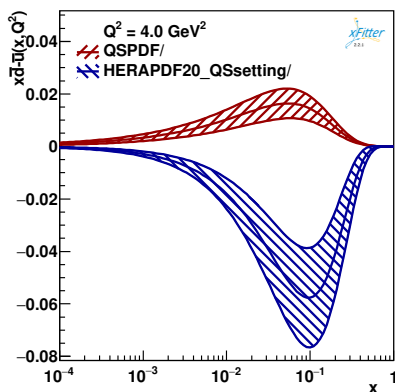


Figure: In blue the benchmark fit with the HERAPDF2.0 parametrisation and in red the fit of QSPDF

Fitting a statistical PDF model

- ✓ We performed a fit a custom PDF parametrisation (QSPDF) against the HERA DIS dataset
- ↑ Acceptable agreement between data and model
- ↑ Fit parameters match a previous attempts at fitting a similar parametrisation
- ↓ This simplest iteration of the parametrisation isn't very competitive against more established models...
- ↑ ...but uses a smaller number of degrees of freedom (8 pars vs 14 of HERAPDF)
- ↑ Qualitative shape of the $\bar{d} - \bar{u}$ distribution reproduced with HERA data only

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Outlook

- Improve the current fit (tuning Q_0 , NNLO theory, resummed theory)
- Modify the parametrisation (relaxing \bar{b} , add transverse potentials) → building a “minimal” parameter set with state-of-the art performance
- Possibility to fit simultaneously unpolarized and polarized PDFs in terms of the same parameters

Thank you for your attention...
but it's not over!

Now it's time for technicalities...

Quark number and momentum sum rules are used to fix three parameters

$$2 = \int_0^1 dx u_v(x, \mu^2), \quad 1 = \int_0^1 dx d_v(x, \mu^2), \quad 1 = \int_0^1 dx x \left[g(x, \mu^2) + \sum_q f_q(x, \mu^2) \right]$$

Usually, these are the normalizations of u_v , d_v and g .

OK for the gluon: momentum sum rule fixes A_g in $xg(x, Q_0^2) = A_g x^{b_g} / (\exp(x/\bar{x}) - 1)$.

However, here u_v and d_v do not have overall normalizations!

$$\begin{aligned} x u_v(x, Q_0^2) &= A \left[X_u^\uparrow h(x; b, \bar{x}, X_u^\uparrow) + X_u^\downarrow h(x; b, \bar{x}, X_u^\downarrow) \right] \\ &\quad - \bar{A} \left[\frac{1}{X_u^\downarrow} h(x; \bar{b}, \bar{x}, -X_u^\downarrow) + \frac{1}{X_u^\uparrow} h(x; \bar{b}, \bar{x}, -X_u^\uparrow) \right] \\ x d_v(x, Q_0^2) &= A \left[X_d^\uparrow h(x; b, \bar{x}, X_d^\uparrow) + X_d^\downarrow h(x; b, \bar{x}, X_d^\downarrow) \right] \\ &\quad - \bar{A} \left[\frac{1}{X_d^\downarrow} h(x; \bar{b}, \bar{x}, -X_d^\downarrow) + \frac{1}{X_d^\uparrow} h(x; \bar{b}, \bar{x}, -X_d^\uparrow) \right] \end{aligned}$$

But A and \bar{A} are the *same for up and down* \rightarrow we can fix them by solving an algebraic system

Quark number sum rules lead to the system

$$\begin{pmatrix} 2 \\ 1 \end{pmatrix} = \begin{pmatrix} K_u & \bar{K}_u \\ K_d & \bar{K}_d \end{pmatrix} \begin{pmatrix} A \\ \bar{A} \end{pmatrix}$$

with

$$K_q = \int_0^1 dx \left[X_q^\uparrow h(x; b, \bar{x}, X_q^\uparrow) + X_q^\downarrow h(x; b, \bar{x}, X_q^\downarrow) \right],$$

$$\bar{K}_q = - \int_0^1 dx \left[\frac{1}{X_q^\downarrow} h(x; \bar{b}, \bar{x}, -X_q^\downarrow) + \frac{1}{X_q^\uparrow} h(x; \bar{b}, \bar{x}, -X_q^\uparrow) \right],$$

Not straightforward to implement in xFitter!

To do so, we implemented a new PDF decomposition in which u, \bar{u}, d, \bar{d} are treated separately

(to be precise, we define them without the “diffractive term” which is added afterwards)

PDF decomposition (vs UvDvUbarDbarS.cc)

```
//  
void UvDvUbarDbarS::atStart(){  
    const YAML::Node node=XFITTER_PARS::getDecompositionNode(_name);  
    //TODO: handle errors  
    par_xuv =getParameterisation(node["xuv"].as<string>());  
    par_xdv =getParameterisation(node["xdv"].as<string>());  
    par_xubar=getParameterisation(node["xubar"].as<string>());  
    par_xdbar=getParameterisation(node["xdbar"].as<string>());  
    par_xs =getParameterisation(node["xs"].as<string>());  
    par_xg =getParameterisation(node["xg"].as<string>());  
}
```

```
void UvDvUbarDbarS::atIteration() {  
    //Enforce sum rules  
    // counting sum-rules for uv and dv  
    par_xuv->setMoment(-1,2.0);  
    par_xdv->setMoment(-1,1.0);  
    // momentum sum-rule  
    // quark part  
    double xsumq=0;  
    xsumq+= par_xuv ->moment(0);  
    xsumq+= par_xdv ->moment(0);  
    xsumq+=2*par_xubar->moment(0);  
    xsumq+=2*par_xdbar->moment(0);  
    xsumq+=2*par_xs ->moment(0);  
    // gluon part  
    par_xg->setMoment(0,1-xsumq);  
}  
std::map<int,double>UvDvUbarDbarS::xfxMap(double x)const  
{  
    double ubar=(*par_xubar)(x);  
    double dbar=(*par_xdbar)(x);  
    double u=(*par_xuv)(x)+ubar;  
    double d=(*par_xdv)(x)+dbar;  
    double s=(*par_xs)(x);  
    double g=(*par_xg)(x);  
    return{
```

```
//  
void QSPDF::atStart(){  
    const YAML::Node node=XFITTER_PARS::getDecompositionNode(_name);  
    //TODO: handle errors  
    par_xu =getParameterisation(node["xu"].as<string>());  
    par_xd =getParameterisation(node["xd"].as<string>());  
    par_xubar =getParameterisation(node["xubar"].as<string>());  
    par_xdbar =getParameterisation(node["xdbar"].as<string>());  
    par_xdiffr=getParameterisation(node["xdiffr"].as<string>());  
    par_xs =getParameterisation(node["xs"].as<string>());  
    par_xg =getParameterisation(node["xg"].as<string>());  
}
```

```
void QSPDF::atIteration() {  
    //Enforce sum rules  
    // counting sum-rules for uv and dv  
    double *normA =XFITTER_PARS::gParameters.at("A");  
    double *normAbar=XFITTER_PARS::gParameters.at("Abar");  
    *normA = 1.;  
    *normAbar = 1.;  
    double Ku = par_xu ->moment(-1);  
    double Kub=-par_xubar->moment(-1);  
    double Kd = par_xd ->moment(-1);  
    double Kdb=-par_xdbar->moment(-1);  
    double DetK = Ku*Kdb - Kub*Kd;  
    *normA = (2*Kdb - Kub)/DetK;  
    *normAbar = (Ku - 2*Kd)/DetK;  
    // momentum sum-rule  
    // quark part  
    double xsumq=0;  
    xsumq+= par_xu ->moment(0);  
    xsumq+= par_xd ->moment(0);  
    xsumq+= par_xubar->moment(0);  
    xsumq+= par_xdbar->moment(0);  
    xsumq+=4*par_xdiffr->moment(0);  
    xsumq+=2*par_xs ->moment(0);  
    // gluon part  
    par_xg->setMoment(0,1-xsumq);  
}  
std::map<int,double>QSPDF::xfxMap(double x)const  
{  
    double diffr=(*par_xdiffr)(x);  
    double ubar=(*par_xubar)(x) + diffr;  
    double dbar=(*par_xdbar)(x) + diffr;  
    double u=(*par_xu)(x) + diffr;  
    double d=(*par_xd)(x) + diffr;  
    double s=(*par_xs)(x);  
    double g=(*par_xg)(x);  
    return{
```

Please output in the final table of parameters also the normalizations found through some rules, ideally with uncertainties!

Parameter	output nf4to5	QS]
'A'	1.0000	
'Abar'	1.0000	
'Ag'	1.0000	
'Atil'	0.1185 ± 0.0069	
'DbarToS'	1.0000	
'Xdd'	0.2741 ± 0.0098	
'Xdu'	0.204 ± 0.026	
'Xud'	0.4327 ± 0.0076	

xFitter computes numerically the integral for the sum rules from $x_0 = 10^{-6}$ to 1 (using logarithmic+linear sampling)

$$\int_0^1 dx x^N f(x, Q_0^2) \simeq \int_{x_0}^1 dx x^N f(x, Q_0^2) \quad (N = 0, 1)$$

For the computation of the sum rules, it is important to account for the small- x behaviour the parametrisation, which is generally a power behaviour

$$f(x, Q_0^2) \stackrel{x \rightarrow 0}{\sim} \alpha x^\beta$$

The integral from 0 to $x_0 = 10^{-6}$ can be better approximated by

$$\int_0^{x_0} dx x^N f(x, Q_0^2) \simeq \alpha \frac{x_0^{\beta+N+1}}{\beta + N + 1}$$

Therefore, extrapolating β and computing α , it is easy to complement the numerical integration above x_0 with the analytical approximate integration below x_0

Useful to avoid values of β that make the PDF non-integrable ($\beta > -1 - N$)

For QSPDFs: $b, \bar{b} > 0$, $\tilde{b} > -1$, $b_g > 0$


```

namespace xfitter{
BasePdfParam::~BasePdfParam(){if(pars)delete[]pars;}
double BasePdfParam::moment(int iMoment)const{
    /// Numeric integration
    /// Simple rule, split log/lin spacing at xsplit=0.1

    const double xsplit = 0.1;
    const double xmin = 1e-6;
    const double xminlog = log10(xmin);
    const double xmaxlog = log10(xsplit);
    const int nlog = 100;
    const int nlin = 100;


    const double xsteplog = (xmaxlog-xminlog)/nlog;
    const double xsteplin = (1.0 - xsplit)/nlin;

    double sum = 0.;
    double x = xmin;

    // log x part:
    for (int i=0; i<nlog; i++) {
        double dx = pow(10,xminlog+(i+1)*xsteplog) - pow(10,xminlog+i*xsteplog);
        double val = (*this)(x+dx/2.)*pow(x+dx/2.,iMoment);
        x += dx;
        sum += dx*val;
    }
    // lin x part:
    for (int i=0; i<nlin; i++) {
        double dx = xsteplin;
        double val = (*this)(x+dx/2.)*pow(x+dx/2.,iMoment);
        x += dx;
        sum += dx*val;
    }
    return sum;
}
}

// extrapolation of the x<xmin part, assuming behaviour f~alpha*x^beta
// here we extrapolate the derivative of the log function in log scale
double logx0 = log(xmin);
double y[3];
double hh, h=log(30); // to be tuned, exp(h)>1/xmin
double f0 = (*this)(xmin);
for(int i=0; i<3; i++){
    hh = h/pow(2.,i);
    volatile double tmp = logx0+hh; // see numerical recipes
    hh = tmp-logx0;
    y[i] = ( log( (*this)(exp(logx0 + hh) ) )-log(f0) ) /hh;
}
double beta = (y[0] - 6*y[1] + 8*y[2])/3.;
double alpha = f0/pow(xmin,beta);
// shift beta to account for Mellin factor x^N
beta += iMoment;
//if beta is too small and negative sum rules are ill-defined
///hopefully setting the output to a large number will kill the normalisation
//constants and force beta to return to nicer values
if(beta<-1) sum += alpha*pow(xmin,beta+1)/(beta+1); // xmin*f0/(beta+1)
else { sum += std::numeric_limits<double>::max(); // to be improved...
      std::cerr<< "Beware, bad beta value"<<std::endl;
    }
}

```



Now it's over.
Thank you.

Backup slides

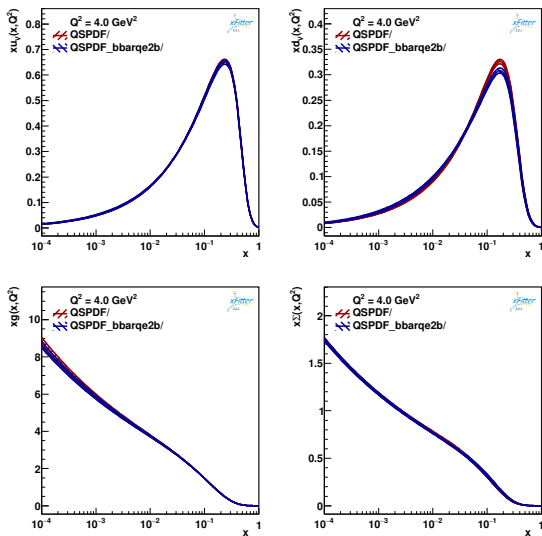


Figure: Effect of different constraint on \bar{b} : $\bar{b} = b$ and $\bar{b} = 2b$

Gluon PDF error in default HERAPDF2.0 fit @NLO

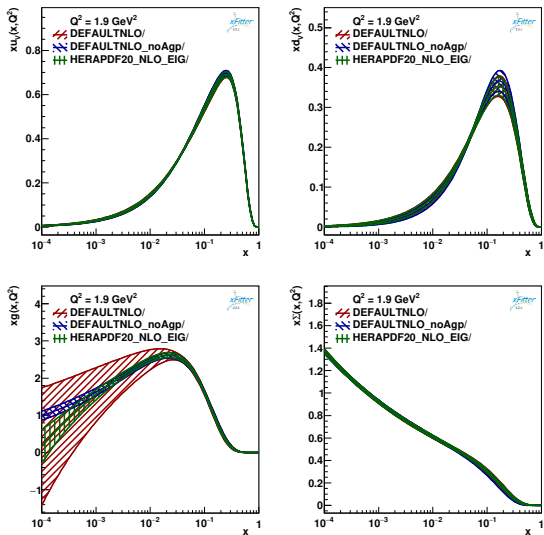


Figure: Large error in the gluon pdf induced by poor determination of $A'_g = 0.23 \pm 0.29$.